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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/524,191	06/05/2006	Christian Bartels	37960-000107/US	3999

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EXAMINER	
YAARY, MICHAEL D	

ART UNIT	PAPER NUMBER
2193	

MAIL DATE	DELIVERY MODE
09/13/2010	PAPER

Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Office Action Summary	Application No.	Applicant(s)	
	10/524,191	BARTELS, CHRISTIAN	
	Examiner	Art Unit	
	MICHAEL YAARY	2193	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE *3* MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

1)☒ Responsive to communication(s) filed on *21 July 2010*.

2a)☒ This action is **FINAL**. 2b)☐ This action is non-final.

3)☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

4)☒ Claim(s) *1-20* is/are pending in the application.

4a) Of the above claim(s) _____ is/are withdrawn from consideration.

5)☐ Claim(s) _____ is/are allowed.

6)☒ Claim(s) *1-20* is/are rejected.

7)☐ Claim(s) _____ is/are objected to.

8)☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

9)☐ The specification is objected to by the Examiner.

10)☐ The drawing(s) filed on _____ is/are: a)☐ accepted or b)☐ objected to by the Examiner.

Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).

Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).

11)☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

12)☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).

a)☐ All b)☐ Some * c)☐ None of:

1.☐ Certified copies of the priority documents have been received.

2.☐ Certified copies of the priority documents have been received in Application No. _____.

3.☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

1) ☐ Notice of References Cited (PTO-892)
2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
3) ☐ Information Disclosure Statement(s) (PTO/SB/08) Paper No(s)/Mail Date _____.
4) ☐ Interview Summary (PTO-413) Paper No(s)/Mail Date. _____ .
5) ☐ Notice of Informal Patent Application
6) ☐ Other: _____.

DETAILED ACTION

1. Claims 1-20 are pending in the application.

Claim Rejections - 35 USC § 102

2. The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

> A person shall be entitled to a patent unless –
>
> (b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

3. Claims 1-20 are rejected under 35 U.S.C. 102(b) as being anticipated by Bartels et al (hereafter Bartels)("Multidimensional Adaptive Umbrella Sampling: Applications to Main Chain and Side Chain Peptide Conformations," Journal of computational Chemistry Volume 18, No 12, Pgs. 1450-1462).

Bartels was cited in the previous office action dated 03/26/2010.

4. **As to claims 1 and 12,** Bartels discloses a method for sampling a state space of a system with states x and a probability density indicating the probability for the system to be in state x by iteratively generating states xi,t and their weighing factors, wherein

the index I is the iteration parameter and the index t distinguishes different states xi,t generated by an iteration i (abstract), the method comprising:

Sampling the state space of the system and performing (pg. 1452, methodology para 1-6),

A first step for selecting an initial sampling distribution function (pg. 1452, methodology para 1-6);

A fifth step for performing an analysis (pg. 1452, methodology para 1-6) and an iteration procedure including a second step for generating Nj states Xj,t by a numerical sampling algorithm and a fourth step for testing one criterion to decide whether to continue the iteration procedure or to stop the iteration procedure and to go to a fifth step in order to perform the analysis using the simulated data, (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2), wherein the iteration further includes a third step determining weighting factors for states xi,t generated so far by using sampling distribution functions determined so far (Pg. 1455, calculation of observables section, columns 1 and 2) and a fitting step for determining a sampling distribution function for the next iteration for states Xi,t generated so far, wherein O(Xi,t) is a function, respectively a property, of the states Xi,t (Pg. 1455, calculation of observables section, columns 1 and 2); and identifying a desired property in the state space of the system based on sampled state space (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2).

5. **As to claim 2,** Bartels discloses the sampling distribution function of at least one iteration is fitted such that it maximizes an objective function preferably defined as a function of local comparisons between the sampling distribution and the product (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2).

6. **As to claims 3 and 13,** Bartels discloses the sampling distribution function of at least one iteration is fitted such that the sampling distribution function is large for at least one stat Xi,t with a large product and tends to be small for states with a small product (methodology, Pg 1452, whole section).

7. **As to claim 4,** Bartels discloses the sampling distribution function of at least one iteration is a function with at least one constraint (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2).

8. **As to claims 5, 14, and 15,** Bartels discloses the sampling distribution function of at least one iteration is the distribution function of the system with constraints or multicanonical distribution function with constraints (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2).

9. **As to claim 6,** Bartels discloses the numerical sampling algorithm of at least one iteration generates correlates states (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2).

10. **As to claim 7,** Bartels discloses the fitting is done by selecting states for which the product has extreme values and by using the selected states to define the region which has extreme values (Pg. 1455, calculation of observables section, columns 1 and 2).

11. **As to claim 8,** Bartels discloses parameters of the sampling distribution function of at least one iteration are determined by a linear least square fit of the logarithm of the un-normalized sampling distribution function to the logarithm of the product (Pg. 1455, calculation of observables section, columns 1 and 2).

12. **As to claim 9,** Bartels discloses the normalization constant of the sampling distribution function of at least one iteration is estimated from the sampled states Xi,t and their weighting factors (Pg. 1455, calculation of observables section, columns 1 and 2).

13. **As to claim 10,** Bartels discloses at least three iterations are done (Pg. 1455, calculation of observables section, columns 1 and 2).

14. **As to claim 11,** Bartels discloses the function is a function of a set of at least two functions (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2).

15. **As to claim 16,** the claim is rejected for similar reasons as claims 2 and 6 above.

16. **As to claim 17,** Bartels discloses the function is a function of a set of at least two functions, including at least one of the following functions:

At least one property for which at least one estimate is derived in the analysis of the fifth step, at least one function that is large for states that must be sampled to ensure transitions between important regions, the inverse of the probability distribution function of at least one property of the system, and the inverse of the probability distribution of the negative logarithm of the distribution function of the system (pg. 1453, Combination of Statistics from Different Simulations, column 1 and 2 and Pg. 1455, calculation of observables section, columns 1 and 2).

17. **As to claims 18-20,** Bartels discloses a computer-readable medium comprising executable program instructions configured to cause a computer to perform the method of claim 1, a computer program, adapted to cause a computer to perform the method of claim 1, and a computer-readable medium comprising the computer program of claim 19 (Inherent in the teachings of Bartels as, a computer-readable medium containing program instructions to be executed in a computer is necessary to perform the calculations.).

Response to Arguments

18. Applicant's arguments filed 07/21/2010 have been fully considered but they are not persuasive. Applicant argues that the Bartels reference does not teach or suggest determining weighting factors for states xi,t generated so far by using sampling distribution functions determined so far. Examiner respectfully disagrees. When taken the broadest reasonable interpretation the teachings of Bartels, as cited above, disclose the claimed limitations. Bartels discloses determining probabilities, ρ as shown. Furthermore, the distributions for other degrees of freedom are obtained using a determined weighing factor; thus a determined weighing factor for states xi,t generated so far by using sampling distribution functions.

Conclusion

THIS ACTION IS MADE FINAL. Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire THREE MONTHS from the mailing date of this action. In the event a first reply is filed within TWO MONTHS of the mailing date of this final action and the advisory action is not mailed until after the end of the THREE-MONTH shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than SIX MONTHS from the mailing date of this final action.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to MICHAEL YAARY whose telephone number is (571)270-1249. The examiner can normally be reached on Mon-Fri 9 a.m.-5:30 p.m.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Lewis Bullock can be reached on 571-272-3759. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see http://pair-direct.uspto.gov. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/M. Y./
Examiner, Art Unit 2193

/Lewis A. Bullock, Jr./
Supervisory Patent Examiner, Art Unit 2193